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Mechanisms of Auger recombination in semiconductor quantum wires

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Abstract. The principal mechanisms of Auger recombination (AR) of nonequilibrium carriers in cylindrical quantum wires (QWRs) are investigated. It is shown that there exist two different Auger recombination mechanisms of (i) quasithreshold and (ii) thresholdless types. These mechanisms originate from the existence of barriers but have different nature. The quasithreshold mechanism is caused by confinement of carriers within the region of a quantum wire which makes the quasi-momentum conservation law approximate and enhances AR process. With increase of the wire radius this process turns to the threshold one. The thresholdless mechanism relates to the violation of the momentum conservation law at the heteroboundary and disappears with the radius tending to infinity.

Introduction

There are two main processes of Auger recombination (AR) in narrow gap semiconductors. The first of them corresponding to recombination of an electron and heavy hole and excitation of another electron is CHCC process. The second CHHS Auger process relates to the transition of a heavy hole to the spin-orbit split-off band. Contrary to bulk semiconductors, the transversal momentum component doesn't conserve in heterostructures thus allowing the thresholdless Auger process to appear [1, 2]. In [3, 4] it was shown that there are three types of AR processes in planar quantum wells (QWs): (i) threshold, (ii) quasithreshold (iii) thresholdless. It is shown that in QWRs there is a similar quasithreshold mechanism becoming 3D Auger process in the limit of a wire with the infinite radius. The AR mechanism of thresholdless type differs from those in a QW because there are two different channels (i) with transfer of a large linear momentum to the excited particle (like in planar QWs) and (ii) with transfer of an angular momentum (which is the only possible channel for quantum dots). These channels have different dependences on barrier heights in the conduction and valence bands.

1 Eigenstates of carriers in a quantum wire

Commonly the basis wave functions in the conduction and valence bands are taken in the form of eigenfunctions of the angular momentum but in the case of cylindrical symmetry it is natural to use another basis [5]:

$$|s\uparrow\rangle,\ |s\downarrow\rangle,\ |p_+\uparrow\rangle,\ |p_+\downarrow\rangle,\ |p_-\uparrow\rangle,\ |p_-\downarrow\rangle,\ |z\uparrow\rangle,\ |z\downarrow\rangle, \tag{1}$$

where $|p_+\rangle = 1/\sqrt{2}|(x+iy)\rangle$, $|p_-\rangle = 1/\sqrt{2}|(x-iy)\rangle$. This procedure excretes eigenfunctions having definite projections of linear and angular momenta on the wire axis. In this basis, dependences of wave functions on the z coordinat, where z-axis is parallel to the axis of the wire, and the axial angle take a simple form. For example the eigenstate in a

bulk semiconductor corresponding to the heavy hole is:

$$\begin{bmatrix} 0 \\ 0 \\ -2iq\,J_{m-3/2}(k\rho)\exp\left(i(m-3/2)\phi\right) \\ k_h J_{m-1/2}(k\rho)\exp\left(i(m-1/2)\phi\right) \\ 0 \\ -k_h J_{m+3/2}(k\rho)\exp\left(i(m+3/2)\phi\right) \\ \sqrt{2}k_h J_{m-1/2}(k\rho)\exp\left(i(m-1/2)\phi\right) \\ 0 \end{bmatrix} \exp(iqz) \tag{2}$$

(where J_m is Bessel function of the mth order). We derive boundary conditions from the continuity of the probability flux density and, following the method elaborated by Burt [6], from integrating Kane's equations across the heteroboundary that give continuity of the following functions:

$$\vec{\psi},\ \frac{d\psi_z}{d\rho},\ m_l^{-1}\mathrm{div}\vec{\psi} \tag{3}$$

where m_l is the mass of light hole in the case of zero constant of spin-orbit interaction [3, 4]. Contrary to situation in QWs [3, 4], the states with different parities cannot be separated even for heavy holes. Therefore, the dispersion equations become rather cumbersome. For example, the simplest one determining the ground state of heavy holes takes the form:

$$\begin{aligned} &\left(\frac{K_{-1}(\kappa_h R)}{J_{-1}(k_h R)} - \frac{K_1(\kappa_h R)}{J_1(k_h R)}\right)\left(\frac{K_2(\kappa_h R)}{J_2(k_h R)} - \frac{K_0(\kappa_h R)}{J_0(k_h R)}\right) \\ &\quad = \frac{4q^2}{\kappa_h^2 k_h^2}\left(k_h\frac{K_{-1}(\kappa_h R)}{J_{-1}(k_h R)} - \kappa_h\frac{K_0(\kappa_h R)}{J_0(k_h R)}\right)\left(k_h\frac{K_2(\kappa_h R)}{J_2(k_h R)} - \kappa_h\frac{K_1(\kappa_h R)}{J_1(k_h R)}\right), \end{aligned} \tag{4}$$

where k and κ are the transversal momentum components inside and outside the wire respectively, K_m is McDonald function of the mth order.

2 Matrix element of Auger recombination

The wave functions of carriers have conserved values of z-components of linear and angular momentum. Performing Fourier transform of Coulomb potential along ρ and ϕ coordinates we obtain:

$$\int_0^{2\pi} d\phi \int_{-\infty}^{\infty} dz \frac{e^{im\phi+iqz}}{|\vec{r}_1 - \vec{r}_2|} = \begin{cases} 4\pi I_m(q\rho_1)K_m(q\rho_2),\ \rho_1 \le \rho_2 \\ 4\pi K_m(q\rho_1)I_m(q\rho_2),\ \rho_1 > \rho_2 \end{cases} \tag{5}$$

(where I_m is the modified Bessel function of the mth order). Obviously, the matrix element of AR automatically yields conservation laws for the linear and angular momentum. We use the approximation $V_c, V_v \ll E_g$, where V_c and V_v are the barrier offsets in the conduction and valence bands, respectively. Procedures of evaluating the matrix element for CHCC and CHHS Auger processes are similar and only CHCC matrix element will be discussed further for the sake of simplicity. For the thresholdless AR process relating to the carrier scattering at the heteroboundary we obtain:

$$\begin{aligned} M^{(1)} = &\frac{8\pi e^2}{\kappa_0(q^2+k_4^2)}\psi_{1s}(R)\psi_{4s}(R)\left\{qRK_{m-1}(qR)\left[\frac{3V_c+V_v}{4E_g}\right]\right. \\ &\left. + mK_m(qR)\frac{3V_c}{4E_g}\right\}\int_0^R \psi_3^*(\rho)\psi_2(\rho)\rho d\rho. \end{aligned} \tag{6}$$

where both the discontinuity of the wave functions and their derivatives give contribution to this matrix element. The first term in the curly brackets, proportional to the linear momentum q, is similar to that existing in QWs. The second one, proportional to angular momentum m, is analogous to the thresholdless mechanism in quantum dots. For the quasithreshold process we have:

$$M^{(2)} = \frac{4\pi e^2}{\kappa_0(q^2 + k_4^2)} \int_0^R \psi_4^*(\rho)\psi_3^*(\rho)\psi_2(\rho)\psi_1(\rho)\rho d\rho. \tag{7}$$

This matrix element, proportional to $\delta(k_4 - k_3)$ in the limit $R \to \infty$, turns to the threshold matrix element in a bulk semiconductor. More detailed analysis of matrix elements of thresholdless and quasithreshold types can be found in [7].

3 Rate of Auger recombination

To calculate the rate of AR in the first order of perturbation theory, the probabilities of transition should be averaged over all initial states of carriers with appropriate weight-occupation numbers and summed over all final states:

$$G = \frac{2\pi}{\hbar} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \langle M^2 \rangle f_1 f_2 (1 - f_3)(1 - f_4)\delta(E_3 + E_4 - E_1 - E_2), \tag{8}$$

here f_1, f_2 are the occupancies of the initial states and f_3, f_4 are those of the final states, $\langle M^2 \rangle$ is the sum of squared Auger matrix elements over spins of the initial and final states. The expression for the rate of Auger process can be derived analytically from (8) but it is rather cumbersome. It is natural to use Auger recombination coefficient C given by:

$$G = Cn^2 p \quad \text{and} \quad G = Cp^2 n$$

for the CHCC and CHHS Auger processes, respectively, where n and p are the 1D densities of electrons and holes. Following [3, 4] we present the coefficient of AR in the form

$$C = C_1 + C_2, \tag{9}$$

where the coefficients C_1 and C_2 correspond to the thresholdless and quasi-threshold Auger processes with the matrix elements M_1 and M_2, respectively. For example, the thresholdless and quasithreshold coefficients for CHCC process are:

$$C_1 \approx \frac{24e^4}{\kappa_0^2} \frac{\hbar^3 \gamma^4}{E_g^5} \frac{F(\Delta_{so}/E_g)}{R^5} \frac{k_c^2 J_0^4(k_c R)}{(J_0^2(k_c R) + J_1^2(k_c R) + K_0^2(\kappa_c R) + K_1^2(\kappa_c R))^2} \times \left\langle \left(\left[\frac{3V_c + V_v}{4E_g} \right]^2 + \frac{m^2}{q^2 R^2} \left[\frac{3V_c}{4E_g} \right]^2 \right) \frac{k_h^2 q^2}{(q^2 + k_4^2)^3 k_f(q)} \right\rangle, \tag{10}$$

$$C_2 \approx \frac{6e^4}{\kappa_0^2} \frac{\hbar^3 \gamma^4}{E_g^5} \frac{F(\Delta_{so}/E_g)}{R^5} \frac{k_c^2 J_0^4(k_c R)}{(J_0^2(k_c R) + J_1^2(k_c R) + K_0^2(\kappa_c R) + K_1^2(\kappa_c R))^2} \times \left\langle \frac{k_h^2}{(q_h^2 + k_h^2) k_f(q)} \frac{\sin^2 (k_f - k_h) R}{(k_f(q) - k_h)^2} \right\rangle, \tag{11}$$

where

$$F(x) = \frac{(1+x/3)(1+x)}{(1+2x/3)(1+x/2)} \frac{1+7x/9+x^2/6}{(1+x/4+x^2/6)}\ ,\ k_f(q) = \sqrt{\frac{2E_g^2}{\hbar^2\gamma^2}\frac{1+\Delta_{so}/2E_g}{1+\Delta_{so}/3E_g} - q^2},$$

the angular brackets denote averaging over the heavy-hole distribution function and k_c is the transversal momentum component of the electron in the ground level.

4 Summary

Our analysis has shown that there exist two different AR mechanisms in semiconductor heterostructures with QWRs: thresholdless and quasithreshold. The thresholdless AR process has two channels. The first of them can be associated with the thresholdless AR process in QWs and the second one can with AR in quantum dots. It is shown that these channels have differrent dependences on barrier heights for electrons and holes in QWRs. The thresholdless coefficient tends to zero and the quasithreshold one becomes the 3D Auger process in the limit of a wire with infinite radius.

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